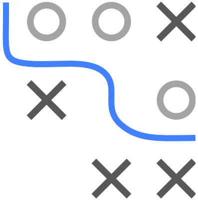
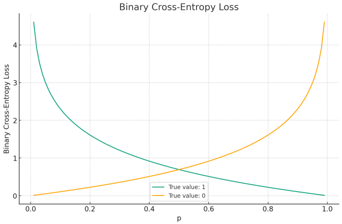
Introduction to Machine Learning



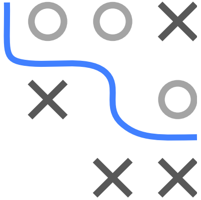
Cross-Entropy and KL



Learning goals

- Know the cross-entropy
- Understand the connection between entropy, cross-entropy, and KL divergence

CROSS-ENTROPY - DISCRETE CASE



Cross-entropy measures the average amount of information required to represent an event from one distribution p using a predictive scheme based on another distribution q (assume they have the same domain $\mathcal{X}$ as in KL).

$$H(p\|q) = \sum_{x \in \mathcal{X}} p(x) \log\left(\frac{1}{q(x)}\right) = -\sum_{x \in \mathcal{X}} p(x) \log\left(q(x)\right) = -\mathbb{E}_{X \sim p}[\log(q(X))]$$

For now, we accept the formula as-is. More on the underlying intuition follows in the content on inf. theory for ML and sourcecoding.

- Entropy = Avg. amount of information if we optimally encode p
- Cross-Entropy = Avg. amount of information if we suboptimally encode p with q
- $DL_{KL}(p\|q)$: Difference between the two
- $H(p\|q)$ sometimes also denoted as $H_q(p)$ to set it apart from KL

CROSS-ENTROPY - DISCRETE CASE / 2

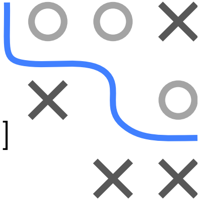
We can summarize this also through this identity:

$$H(p\|q) = H(p) + D_{KL}(p\|q)$$

This is because:

$$\begin{aligned}
H(p) + D_{KL}(p\|q) &= -\sum_{x \in \mathcal{X}} p(x) \log p(x) + \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)} \\
&= \sum_{x \in \mathcal{X}} p(x)(-\log p(x) + \log p(x) - \log q(x)) \\
&= -\sum_{x \in \mathcal{X}} p(x) \log q(x) = H(p\|q)
\end{aligned}$$

CROSS-ENTROPY - CONTINUOUS CASE



For continuous density functions $p(x)$ and $q(x)$:

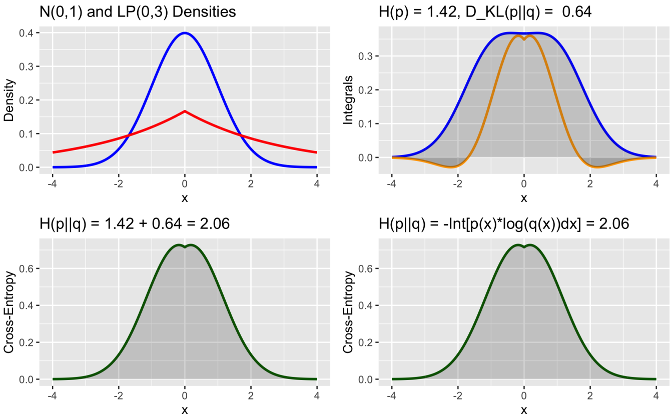
$$H(p\|q) = \int p(x) \log\left(\frac{1}{q(x)}\right) dx = -\int p(x) \log\left(q(x)\right) dx = -\mathbb{E}_{X\sim p}[\log(q(X))]$$

- It is not symmetric.
- As for the discrete case, $H(p\|q) = h(p) + D_{KL}(p\|q)$ holds.
- Can now become negative, as the $h(p)$ can be negative!

CROSS-ENTROPY EXAMPLE

Let $p(x) = N(0,1)$ and $q(x) = LP(0,3)$. We can visualize

$$H(p\|q) = H(p) + D_{KL}(p\|q)$$



CROSS-ENTROPY EXAMPLE

Let $p(x) = LP(0,3)$ and $q(x) = N(0,1)$. We can visualize

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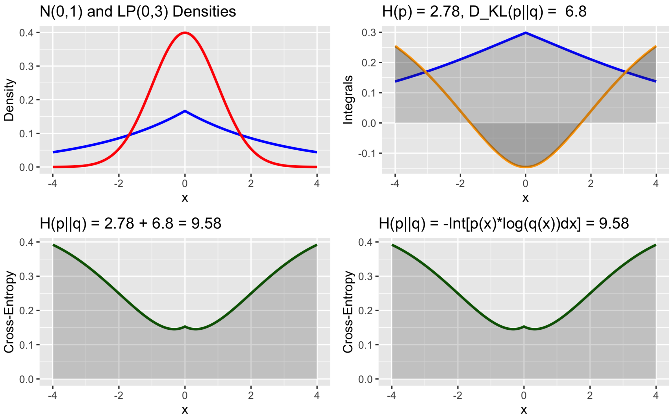

PROOF: MAXIMUM OF DIFFERENTIAL ENTROPY

Claim: For a given variance, the continuous distribution that maximizes differential entropy is the Gaussian.

Proof: Let $g(x)$ be a Gaussian with mean μ and variance σ^2 and $f(x)$ an arbitrary density function with the same variance. Since differential entropy is translation invariant, we can assume $f(x)$ and $g(x)$ have the same mean.

The KL divergence (which is non-negative) between $f(x)$ and $g(x)$ is:

$$\begin{aligned} 0 \leq D_{KL}(f \| g) &= -h(f) + H(p \| q) \\ &= -h(f) - \int_{-\infty}^{\infty} f(x) \log(g(x)) dx \end{aligned} \tag{1}$$

PROOF: MAXIMUM OF DIFFERENTIAL ENTROPY / 2

The second term in (1) is,

$$
\begin{aligned}
\int_{-\infty}^{\infty} f(x)\log(g(x))dx &= \int_{-\infty}^{\infty} f(x)\log\left(\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}\right)dx \\
&= \int_{-\infty}^{\infty} f(x)\log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)dx + \log(e)\int_{-\infty}^{\infty} f(x)\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)dx \\
&= -\frac{1}{2}\log\left(2\pi\sigma^2\right) - \log(e)\frac{\sigma^2}{2\sigma^2} = -\frac{1}{2}(\log\left(2\pi\sigma^2\right) + \log(e)) \\
&= -\frac{1}{2}\log\left(2\pi e\sigma^2\right) = -h(g)\,, \qquad (2)
\end{aligned}
$$

where the last equality follows from the normal distribution example of the entropy chapter. Combining (1) and (2) results in

$$h(g) - h(f) \geq 0$$

with equality when $f(x) = g(x)$ (following from the properties of Kullback-Leibler divergence).